Atomic data and collisional-radiative model for Beryllium and its ions

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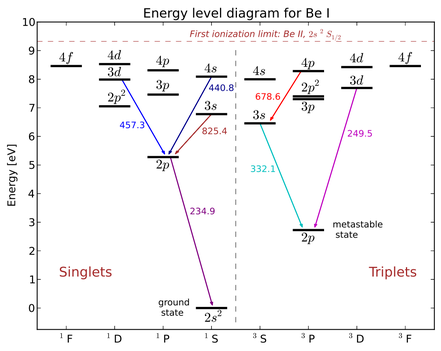
Introduction

Be is foreseen as a plasma-facing material in the main chamber of ITER. For interpretation of spectroscopic measurements and for modelling of the Be impurity transport in the edge and divertor plasma, collisional atomic data (cross sections of elementary processes) are required. The "effective" rate coefficients given in existing atomic databases (e.g. ADAS) are sometimes insufficient for applications. Due to high toxicity of Be the experimental cross sections are practically unavailable in the literature. As a rule the most accurate theoretical methods, such as convergent close-coupling (CCC) or the R-matrix with pseudostates (RMPS) demand very large computation time (especially at intermediate energies when continuum coupling effects are important). For the relatively fast calculation simpler but accurate enough methods such as K-matrix can be used.

Convergent close-coupling calculations for Be I

- All transitions with $n \leq 4$ for collision energies $E \leq 400$ eV included.
- 293 Laguerre basis states in the new, 108 states in the old calculations [*D. Fursa & I. Bray, JPB: At. Mol. Opt. Phys. 30 (1997)*]
- For energies below 10 eV (relative to the ground state) - 10 partial waves, and 16 - above. Extrapolation to infinity done using the Born approximation.



Code ATOM

Computes atomic characteristics:

- Radiative: f, A, σ (photoionization/recombination), autoionization
- Collisional: σ, $\langle v\sigma \rangle$ of excitation, ionization by electrons and protons

Included in ATOM:

- For wave functions: exchange, scaled potential, core polarization
- For collisions: Coulomb field, exchange, normalization, configuration interaction (with optional matrix of eigenvectors)

One-electron radial equation:

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + 2\frac{\zeta_c(r/\omega)}{r} + \varepsilon\right] P_{nl}(r) = -2\sum_{\gamma}\frac{\zeta_{e\gamma}(r/\omega)}{r} P_{\gamma}(r/\omega)$$

- For $\varepsilon(nlSL)$ the experimental bound energy is used
- The scale parameter ω is an eigenvalue such that $P(0) = 0$ and $P(r) \underset{r\to\infty}{\sim} \exp(-r\sqrt{\varepsilon})$. In this case ε gives the correct asymptotic behavior of $P(r)$.

K-matrix method (transitions between terms)

- A chosen list of atomic states (basis) is used as an input information.
- For all pairs of states (a_i, a_f : $E_i < E_f$) from the basis, for a set of partial waves (λ_i, λ_f) of the outer electron and for total angular momenta S_T, L_T the transition amplitudes K^B are calculated in Born (for neutrals) or Coulomb-Born (for ions) approximation with exchange between the incident and target electrons.
- From transition amplitudes the full matrix $\mathbf{K}^B$ is constructed. The final unitary scattering matrix $\mathbf{S}$ is obtained according to the matrix equation

$$\mathbf{S} = \frac{\mathbf{I} + i\mathbf{K}^B}{\mathbf{I} - i\mathbf{K}^B}$$

- The cross section is expressed in terms of S-matrix:

$$\sigma\left(S_i L_i - S_f L_f\right) = \frac{1}{2k_i^2}\sum_{S_T L_T \lambda\lambda'}\frac{[S_T L_T]^2}{[S_i L_i]^2}\left|S_{\Gamma_i\Gamma_f} - \delta_{\Gamma_i\Gamma_f}\right|^2$$

The method takes into account:

- Normalization (electron flux conservation)
- Step transitions (e.g., $2s - 2p - 3d$)
- Other less straightforward consequences of the channel interaction

K-matrix method (basic formulae)

The full set of quantum numbers $\Gamma = as\lambda S_T L_T$. Usually $a = \gamma_c S_c L_c nlSL$. The elements of K-matrix are equal to the matrix elements of interaction:

$$K^B_{\Gamma_i\Gamma_f} = \left\langle \Gamma_i | \hat{V} | \Gamma_f \right\rangle = \sum_\kappa A_\kappa \left(R'_\kappa - B_S R''_\kappa\right), \quad \hat{V} = \frac{1}{|\mathbf{r}-\mathbf{r}'|} = \sum_\kappa P_\kappa(\cos\theta)\frac{r_<^\kappa}{r_>^{\kappa+1}}$$

The direct R'_κ and exchange R''_κ radial integrals are expressed through radial functions P_l and F_λ of the optical and outer electron, respectively:

$$R'_\kappa = \chi(l_i l_f \lambda_i \lambda_f \kappa)\int_0^\infty\int_0^\infty F_{\lambda_i}(r') P_{l_i}(r'')\frac{r_<^\kappa}{r_>^{\kappa+1}} P_{l_f}(r'') F_{\lambda_f}(r') dr'' dr'$$

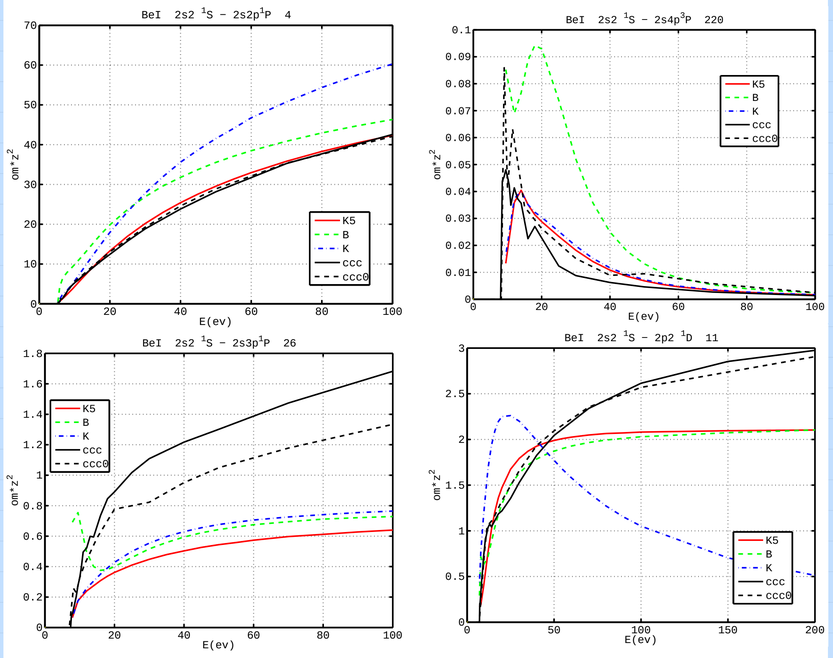
$$R''_\kappa = \sum_{\kappa''}(-1)^{\kappa+\kappa''}\left[\kappa\kappa''\right]^2 \begin{Bmatrix} \kappa & l_i & l_f \\ \kappa'' & \lambda_i & \lambda_f \end{Bmatrix} R^e_{\kappa''}$$

$$R^e_{\kappa''} = \chi\int_0^\infty\int_0^\infty \tilde{F}_{\lambda_i}(r') P_{l_i}(r'')\frac{r_<^\kappa}{r_>^{\kappa+1}}\left(1 - cr_>\delta_{\kappa'',0}\right) P_{l_f}(r') \tilde{F}_{\lambda_f}(r'') dr'' dr'$$

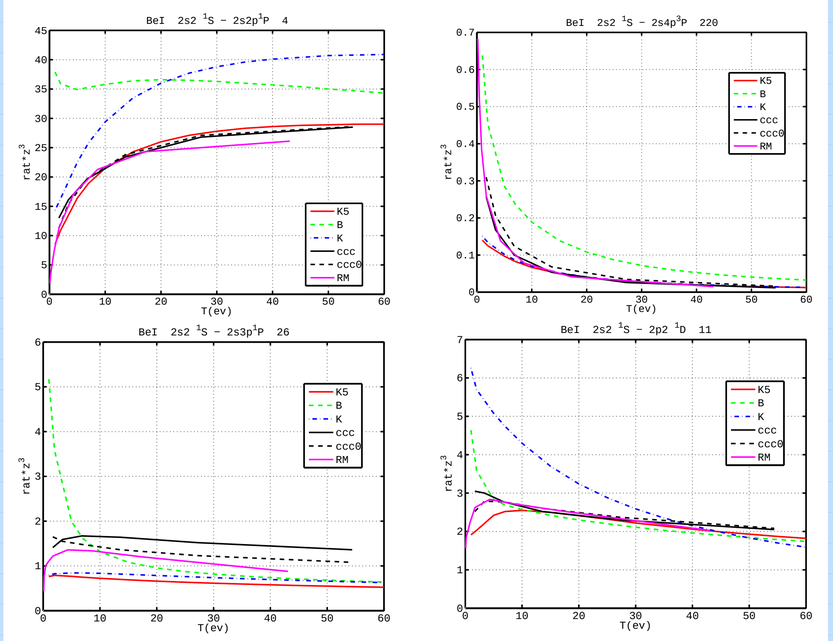
Comparison between CCC and K-matrix for Be I

- Good agreement was obtained for dipole transitions, if oscillator strength f is not very small. We note also the significant influence of the configuration mixing. For intercombination transitions the difference is somewhat larger because the exchange is normally more sensitive to the used approximations.
- Poor agreement was found in cases of very strong configuration interaction when the description of atomic structure used in ATOM can be inadequate and for transitions with extremely small f-values for which the cancellation effects are important.
- Some questionable cases, e.g. the transition $2s^2\ ^1S \rightarrow 2p^2\ ^1D$. Two mechanisms are possible: the "step" $2s^2\ ^1S \rightarrow 2s2p\ ^1P \rightarrow 2p^2\ ^1D$ (with asymptotic $\Omega \propto \frac{1}{E}$) and the quadrupole transition ($2p^2\ ^1S \rightarrow 2p^2\ ^1D$) due to configuration interaction $2s^2\ ^1S + 2p^2\ ^1S$ (the asymptotic $\Omega \rightarrow$ const). The increasing CCC collision strength can indicate the non-orthogonality of $2p^2\ ^1S$ and $2p^2\ ^1D$ states.
- In most cases the agreement between rate coefficients is usually much better than for cross sections.

Electron impact excitation of Be I: collision strengths



Electron impact excitation of Be I: rate coefficients



Collisional-radiative model

The following 80 states were included in CRM:

- Be I: $2s^2\ ^1S$; $2snl\ ^1L, ^3L$, $L = l$, $n = 2-4$, all l; $2p^2\ ^1D, ^3P$ (19 terms)
- Be II: $1s^2 nl\ ^2L$, $L = l$, $n = 2-6$, all l (20 terms)
- Be III: $1s^2\ ^1S$; $1snl\ ^1L, ^3L$, $L = l$, $n = 2-4$, all l (19 terms)
- Be IV: $nl\ ^2L$, $L = l$, $n = 1-6$, all l (21 terms)
- Be V (bare nucleus): (1 state)

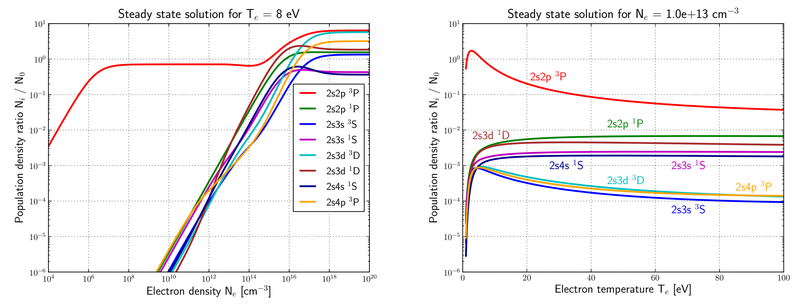
Atomic data:

- Energies of levels and radiative transition probabilities A_{ij} were taken from NIST database.
- A new improved set of CCC excitation and ionization cross sections for Be I as well as CCC data [*A. Starobinets et al. Physica Scripta 67 (2003) 500*] for Be II were used. For selected transitions in Be I, Be II and for ions Be III, Be IV the K-matrix (for excitation) and the normalized Born (for ionization) cross sections were computed by the code ATOM.
- The partial photorecombination cross sections for all ion stages were calculated by the ATOM code.
- Dielectronic recombination rates were taken from [*P. Mazzotta et al. Astron. Astrophys. Suppl. Ser. 133 (1998) 403*].
- For inverse processes (de-excitation and three-body recombination) the principle of detailed balance was used.

The collisional-radiative code NOMAD:

- (Non-Maxwellian) time-dependent collisional-radiative code for calculation of ionization balance, plasma emission characteristics, radiative power losses, etc.
- Account of plasma effects (opacity, ionization potential lowering)
- Applications: diagnostics of various plasmas (laser-produced, astrophysical, fusion)

Steady-state dependencies on Ne and Te for Be I

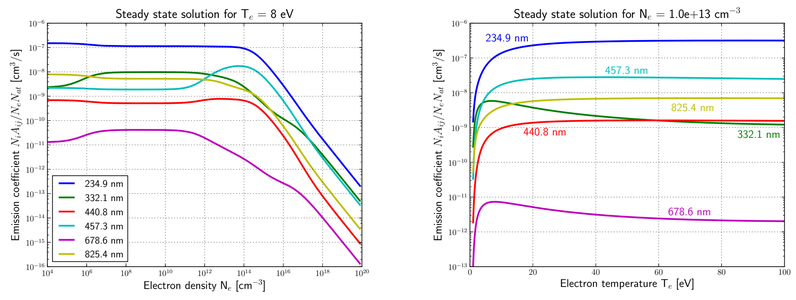


For electron density three regions are present (Te = 8 eV):

- Corona region $N_e \leq 10^6$ cm^{-3}: all populations of excited states (including metastable) are proportional to electron density
- Intermediate density region $10^8 \leq N_e \leq 10^{11}$ cm^{-3}: the population of metastable does not depend on N_e and is still $\propto N_e$ for other excited states
- High density region $N_e \geq 10^{18}$ cm^{-3}: population densities are determined by collisions and independent on N_e

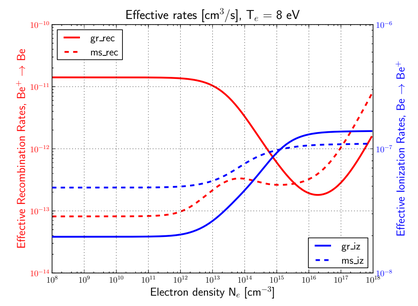
Singlets and triplets behave differently with Te:

- Relative populations of singlet excited states have similar temperature dependence as excitation rate from ground state
- Triplet excited states are populated through the metastable level and relative populations depend on T_e similar to excitation rate from ground state to metastable



Effective ionization and recombination rate coefficients

- Quasi-steady-state approximation: $dN_i/dt = 0$ for the excited states except for ground and metastable states.
- The excited states make essential contribution to the effective rates.
- Nonmonotonic recombination rate due to competition between the recombination to and the collisional ionization from excited states.
- The effective ionization rate increases monotonically and becomes saturated at high N_e.



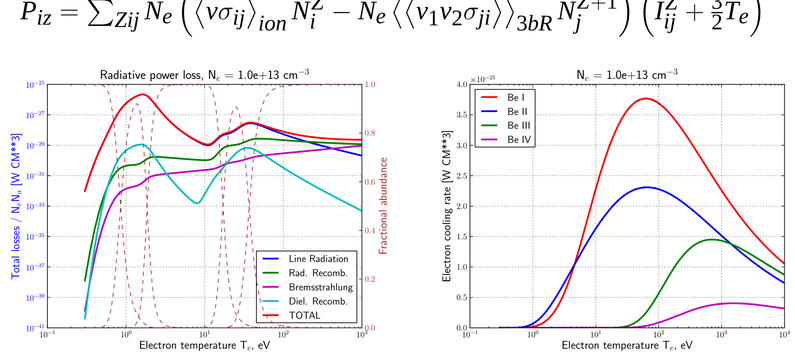
Radiative power losses and cooling rates

The radiation losses include the following contributions:

- Line radiation (cascades): $P_{em} = \sum_{Zij} N_i^Z A_{ij}^Z \Delta E_{ij}^Z$
- Radiative and dielectronic recombination: $P_{rec} = \sum_{Zij} N_e\left(\langle v\sigma_{ji}\rangle_{rr}\left(I_{ij}^Z + \frac{3}{2}T_e\right) + \langle v\sigma_{ji}\rangle_{dr}\Delta\bar{E}_j^{Z+1}\right) N_j^{Z+1}$
- Acceleration of electrons by the ions (bremsstrahlung): $P_{br} \propto N_e^2 Z_{eff}\sqrt{T_e}, \quad Z_{eff} = \sum_k N_k Z_k^2 / N_e$

Electron cooling rate by excitation and ionization:

- Collisional excitation and deexcitation: $P_{ex} = \sum_{Zij} N_e\left(\langle v\sigma_{ij}\rangle_{ex} N_i^Z - \langle v\sigma_{ji}\rangle_{dex} N_j^Z\right)\Delta E_{ij}^Z$
- Ionization and three-body recombination: $P_{iz} = \sum_{Zij} N_e\left(\langle v\sigma_{ij}\rangle_{ion} N_i^Z - N_e\langle\langle v_1 v_2 \sigma_{ji}\rangle\rangle_{3bR} N_j^{Z+1}\right)\left(I_{ij}^Z + \frac{3}{2}T_e\right)$



Conclusion

- Electron impact excitation and ionization cross sections were calculated by two independent methods: the sophisticated Convergent Close-Coupling (for Be I) and Coulomb-Born-Exchange (for all Be ions). The comparison of cross sections for Be I demonstrates reasonable agreement. The CBE results for H, He, Li, Be and Be$^+$ are presented on IAEA website: http://www-amdis.iaea.org/Atom_AKM/. Similar calculations (possibly including fine structure transitions) can easily be done for other light (small-electron) elements (e.g., for alkali or alkaline earth atoms and their isoelectronic ions).
- Collisional-radiative model for Be ions including the new improved set of CCC excitation and ionization cross sections was constructed. Fractional ion abundances, electron cooling rates, radiative power losses and effective emission coefficients were calculated as functions of electron temperature in a wide range of plasma densities by the NOMAD code.